On CP, LP and other piecewise perturbation methods for the numerical solution of the Schrödinger equation

Veerle Ledoux and Marnix Van Daele

Zeitschrift für angewandte Mathematik und Physik: Volume 62, Issue 6 (2011), Page 993-1011

Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Volume 62, Number 6, 993-1011, DOI: 10.1007/s00033-011-0158-8

On CP, LP and other piecewise perturbation methods for the numerical solution of the Schrödinger equation

Veerle Ledoux and Marnix Van Daele

Abstract. The piecewise perturbation methods (PPM) have proven to be very efficient for the numerical solution of the linear time-independent Schrödinger equation. The underlying idea is to replace the potential function piecewisely by simpler approximations and then to solve the approximating problem. The accuracy is improved by adding some perturbation corrections. Two types of approximating potentials were considered in the literature, that is piecewise constant and piecewise linear functions, giving rise to the so-called CP methods (CPM) and LP methods (LPM). Piecewise polynomials of higher degree have not been used since the approximating problem is not easy to integrate analytically. As suggested by Ixaru [21], this problem can be circumvented by using another perturbative approach to construct an expression for the solution of the approximating problem. In this paper, we show that there is, however, no need to consider PPM based on higher order polynomials, since these methods are equivalent to the CPM. Also LPM is equivalent to CPM, although it was sometimes suggested in the literature that an LP method is more suited for problems with strongly varying potentials. We advocate that CP schemes can (and should) be used in all cases, since it forms the most straightforward way of devising PPM and there is no advantage in considering other piecewise polynomial perturbation methods.

Mathematics Subject Classification (2010). 65L15; 65Z05; 34B09; 34L16.

Keywords. Schrödinger, eigenvalue problem, perturbation, CP method.

Veerle Ledoux is a Postdoctoral Fellow of the Research Foundation-Flanders (FWO).

1. Introduction

We consider the numerical solution of the one-dimensional time-independent Schrödinger problem

$$y'' = (V(x) - E)y, \quad a \leq x \leq b. \tag{1.1}$$

The problem can both be defined as an initial value probem or as a boundary value problem.

The efficient solution of the stationary Schrödinger initial value problem (1.1) is for example crucial in the simulation of the electron transport in nanoscale semiconductor devices (see [4, 5, 6]). In such applications, macroscopic quantitities such as the electron density or the current density are computed as an integral over the energy variable of single state quantities. For instance the electron density n is derived from the wave function y:

$$n(x) = \int |y(x)|^2 f(E) dE$$

where f represents the injection statistics of the electrons, described by the Fermi-Dirac or the Boltzmann distribution function. Thus, the Schrödinger equation (1.1) has to be solved repeatedly for different E in order to compute the quantity n and consequently efficient methods for the solution of (1.1) lead to a considerable gain in the simulation time.

When boundary conditions are imposed on the Schrödinger equation, the boundary value problem can be seen as a Sturm-Liouville problem in which the eigenvalues E and the associated eigenfunctions y are sought. Schrödinger and Sturm-Liouville eigenvalue problems arise in quantum physics, quantum chemistry, transporty theory, geophysical applications, and vibration and heat flow problems in mechanical engineering. They also arise from the standard separation of variables method applied to a linear partial differential equation, and in connection with the inverse scattering transform for solving nonlinear partial differential equations. Most eigenvalue problems are not analytically solvable and computationally efficient approximation techniques are of great applicability. The numerical computation of the eigenvalues and eigenfunctions can however be a computationally challenging task. In fact, many standard numerical methods involve the approximation of the corresponding eigenfunctions by piecewise polynomials and are therefore inefficient for the computation of higher eigenvalues which have severely oscillatory eigenfunctions. There have e.g. been many developments in the basic approach of reduction to a matrix eigenproblem using finite differences and finite elements [3, 35, 43]. These matrix methods are simple to set up but their main disadvantage is the difficulty in providing high order approximations with uniform error bounds. In this respect, shooting methods perform much better (see [40]).

Shooting methods are based on the reduction of the boundary value problem to the solution of an initial value problem. The differential equation is solved as an initial value problem over the range $[a, b]$ for a succession of trial values of E which are adjusted till the boundary conditions at both ends

can be satisfied at once, at which point we have an eigenvalue. Shooting methods based on standard initial-value library codes are not very effective for the Schrödinger problem. The highly oscillatory behaviour of the solutions corresponding to high eigenvalues, forces a naive integrator to take increasingly smaller steps. Better results are obtained using methods based on coefficient approximation since, for such methods, the step size is not restricted by the oscillations in the solution. The idea is to replace the potential function $V(x)$ by simpler approximations $\bar{V}(x)$ (usually low degree polynomials) and then to solve the approximating problem. There is a substantial literature on such methods, dating back at least to the early seventies: [9, 7, 16, 36, 42, 37, 38]. Except voor Gordon [9], who used linear functions, the early references all used piecewise constant approximations. The replacement of $V(x)$ by $\bar{V}(x)$ is made piecewisely, i.e., the integration interval $[a, b]$ is first partitioned

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b$$

and a suitable $\bar{V}(x)$ is introduced on each subinterval $[x_{i-1}, x_i]$.

As Pruess showed [37], when approximating V by a piecewise polynomial $\bar{V}$ the best option is to approximate V over each mesh interval by a polynomial that interpolates V at the Gauss-Legendre points. This approach is equivalent to developing V over shifted Legendre polynomials. Piecewise polynomial interpolants of degree m give then rise to an $O(h^{2m+2})$ error (see [40]). When a piecewise constant approximation is used ($m = 0$) the approximating problem can be integrated explicitly in terms of trigonometric/hyperbolic functions. Piecewise constant approximation was applied in some successful Sturm-Liouville solvers for second order [34, 39, 41] and higher order problems [10, 11, 12]. Piecewise linear approximations ($m = 1$) lead to solutions which are expressed in terms of the Airy functions [2, 9]. In practice, it is difficult to use the solutions of a problem with a piecewise polynomial $\bar{V}$ of a degree higher than one ($m > 1$) as approximations for the solutions of a Schrödinger problem, since the approximating problem may be no easier to solve numerically than the original. This means that for a long time only second and fourth order coefficient approximation methods were used. A solution was offered by a technique from mathematical physics: the perturbation approximation. The idea is to take for $\bar{V}$ only the potentials for which the two independent solutions have known, analytic forms which can be calculated efficiently. To further improve the accuracy, some corrections are computed from the perturbation $\Delta_V(x) = V(x) - \bar{V}(x)$ using a perturbative procedure. Such a perturbative approach for a Schrödinger type equation was discussed in detail by Ixaru in [17] and used in the development of a general family of (high order) piecewise perturbation methods (PPM) (see [18, 22, 29]).

A PPM is well suited for the repeated solution of the initial value problems which appear in the shooting procedure. As shown in [22, 30], an E-independent mesh can be computed which is then (re)used in all eigenvalue computations which makes the actual shooting process very fast. The step sizes in the mesh are typically much larger than the solution wavelength,

which means that also accurate approximations for higher eigenvalues are computed surprisingly fast. The PPM allow a simple interval truncation algorithm for singular and infinite problems: evaluating the coefficients only at the Legendre nodes effectively regularizes the problem. The PPM formed the basis for the Matlab software package Matslise [30] and were generalized to systems of coupled Schrödinger equations in [19, 31]. These PPM schemes for large systems of coupled channel Schrödinger equations can also be employed in the numerical solution of problems in more than one dimension and problems with a time-dependent Hamiltonian (see [24, 28]). The piecewise perturbation or coefficient approximation method can e.g. be applied to the linear ODE system which arises after space discretization of a time-dependent Schrödinger equation.

Two ways of implementing a PPM were considered in the literature. As shown in [22], if on each mesh interval $\bar{V}(x)$ is taken as a constant and $V(x)$ is a polynomial, then the perturbation corrections have simple analytic forms. The numerical methods obtained on this basis are referred to as forming the CPM (short for constant (based) perturbation method) family. A piecewise line for $\bar{V}(x)$ leads to a LPM (linear perturbation method), see [27, 21]. Although a higher degree piecewise polynomial approximation $\bar{V}(x)$ is closer to the exact potential $V(x)$, one has never succeeded in constructing a PPM with a higher degree polynomial $\bar{V}(x)$ which is more efficient than a CPM or an LPM scheme. The reason is that the analytic integration of the approximating problems is not easy. We will show in the present paper, however, that even if one would have an efficient procedure to compute the solutions of the approximating problem, this would lead us to a scheme which is equivalent to a CPM or an LPM scheme. In fact all piecewise perturbation methods based on piecewise polynomial approximations of degree larger than zero are equivalent to a CPM scheme. Also the LPM offer no advantage over CPM schemes, although it was suggested in literature that they may be more suited on mesh intervals where the potential exhibits strong variation.

As shown in [8], the PPM fit into the framework of modified (Magnus or Neumann) integral series methods which were specially designed to integrate highly oscillatory systems. Very similar ideas were also used to compute the highly oscillatory solution of singularly perturbed Schrödinger equations with time-dependent Hamiltonian in [25, 26]. As described in [13, 14], application of a modified integral series method combines two ideas: a local change of variables with respect to a fast-rotating frame of reference induced by the nearby problem with constant coefficients and the application of a Magnus or Neumann series method. The integrals in the series terms are replaced by Filon quadrature which respects high oscillation (see [15]). As shown in [32, 33], applying a modified Neumann or Magnus method in combination with a Filon quadrature rule to a problem of the form (1.1), involves the computation of the exact solution of the problem with constant potential $\bar{V}$ and the replacement of $V(x)$ by polynomial approximations to allow the evaluation of the resulting series terms. This illustrates that, next to the PPM,

modified Magnus or Neumann schemes also form a natural extension of the coefficient approximation idea to higher order methods. A modified Neumann scheme applied on the problem (1.1) corresponds in fact even exactly to the application of a CPM sheme. When only the first term in the Neumann series is retained, one has exactly the second order method corresponding to a piecewise constant approximation of the potential. Higher order methods are obtained by including more Neumann terms. In [8] it was shown that each extra Neumann term equals a correction term in a CPM. In [14] a modified Neumann scheme (or equivalently a CPM) was applied in a PDE setting, in particular in the semidiscretization of the linear time-dependent Schrödinger equation.

In order not to unnecessary complicate things, we will only consider the implementation of the different PPM schemes here in the context of the time-independent form (1.1) of the Schrödinger equation. How the PPM and related ideas can be extended to time-dependent problems or problems with more dimensions has been described elsewhere and is to a large extent independent of the specific coefficient approximation method used and is consequently not important for the main message of this paper. We first give more details about coefficient approximation methods in section 2. The perturbation approximation ideas are then discussed in section 3. In the literature, different approaches have been presented which can be followed to construct a PPM leading to different subclasses of PPM. We will show here that, when it comes however to the implementation into a practical scheme, these different approaches lead to the same algorithm and that there is e.g. no need to make a distinction between CPM and LPM. This will be illustrated in section 4.

2. Coefficient approximation methods

We focus on the initial value problem

$$y'' = (V(x) - E)y\,, \quad x \in [a, b]\,, \tag{2.1}$$

as it appears in the shooting procedure to solve the eigenvalue problem. Initial conditions are given in one of the endpoints, e.g.

$$y(a) = y_0, \quad y'(a) = y_0'\,. \tag{2.2}$$

We assume that the potential function $V(x)$ is a well behaved (i.e. real, bounded and continuous) function and E, the energy, is a constant. Let us focus on the current mesh interval $[x_{i-1}, x_i]$ of steplength h_i. Our aim is to construct an algorithm which propagates the solution from one endpoint of this interval x_{i-1} to the other endpoint x_i. We introduce the variable $\delta = x - x_{i-1}$, $\delta \in [0, h_i]$ and denote generically $X = x_{i-1}$ and $h = h_i$. The local one-step problem is then

$$y''(X + \delta) = (V(X + \delta) - E)y(X + \delta)\,, \quad \delta \in [0, h] \tag{2.3}$$

with some known initial conditions $y(X) = \alpha$, $y'(X) = \beta$.

We consider two particular solutions of (2.3), $u(\delta)$ and $v(\delta)$ which satisfy the initial conditions

$$u(0) = 1,\ u'(0) = 0, \tag{2.4}$$

and

$$v(0) = 0,\ v'(0) = 1. \tag{2.5}$$

The functions u and v are linear independent and their wronskian

$$W(u, v) = uv' - u'v \tag{2.6}$$

is equal to 1. It follows that a solution of (2.3) has the form

$$y(X + \delta) = c_1 u(\delta) + c_2 v(\delta), \tag{2.7}$$

where c_1 and c_2 are two constants. From (2.4) and (2.5) we know that $c_1 = y(X)$ and $c_2 = y'(X)$. The solution of Eq. (2.3) can thus be written in matrix form as follows

$$\begin{bmatrix} y(X+\delta) \\ y'(X+\delta) \end{bmatrix} = \begin{bmatrix} u(\delta) & v(\delta) \\ u'(\delta) & v'(\delta) \end{bmatrix} \begin{bmatrix} y(X) \\ y'(X) \end{bmatrix}. \tag{2.8}$$

Taking the inverse of this formula, we obtain

$$\begin{bmatrix} y(X) \\ y'(X) \end{bmatrix} = \begin{bmatrix} v'(\delta) & -v(\delta) \\ -u'(\delta) & u(\delta) \end{bmatrix} \begin{bmatrix} y(X+\delta) \\ y'(X+\delta) \end{bmatrix}. \tag{2.9}$$

The role of the functions u and v is thus to propagate the (exact) solution from X to $X + \delta$ and vice versa. Therefore u and v are called exact *propagators* (see [17]). It is clear that the knowledge of the propagators u, v and their first derivatives u', v' is sufficient to advance the solutions in both directions. However, analytic forms of these u and v are known only for a restricted number of expressions for the function $V(x)$, let such functions be denoted by $\bar{V}(x)$. The idea behind coefficient approximation is to replace the coefficient $V(x)$ piecewisely by a $\bar{V}(x)$. That is, we associate to Eq. (2.3) an equation of the same form

$$y''(X + \delta) = \left[\bar{V}(X + \delta) - E\right] y(X + \delta), \quad \delta \in [0, h], \tag{2.10}$$

which is called the *reference equation*. The so-called *reference potential* $\bar{V}(x)$ is chosen in such a way that this equation has known analytic solutions and is typically a low degree polynomial. In particular we are interested in the two solutions $\bar{u}(\delta)$ and $\bar{v}(\delta)$ which are the propagators of Eq. (2.10) and form approximations for the unknown propagators $u(\delta)$ and $v(\delta)$.

2.1. Constant approximation method

The simplest coefficient approximation method is based on a piecewise constant approximation of the potential function, i.e. $\bar{V}(\delta) = \bar{V}$. The following

expressions are then obtained for the propagators:

$$u(\delta) \approx \bar{u}(\delta) = \eta_{-1}(Z(\delta)) \tag{2.11}$$
$$v(\delta) \approx \bar{v}(\delta) = \delta\eta_0(Z(\delta)) \tag{2.12}$$
$$u'(\delta) \approx \bar{u}'(\delta) = Z(\delta)\eta_0(Z(\delta))/h \tag{2.13}$$
$$v'(\delta) \approx \bar{v}'(\delta) = \eta_{-1}(Z(\delta)) \tag{2.14}$$

where $Z(\delta) = (\bar{V} - E)\delta^2$ and the functions η_{-1} and η_0 as defined in the Appendix. Piecewise constant approximation was applied in a shooting process by Pruess and Fulton in their well-known Sturm-Liouville software package [39]. Choosing $\bar{V} = V(X + h/2)$ leads to a method of order two.

2.2. Linear approximation method (Gordon's method)

Gordon was the first to consider the use of piecewise linear approximations to the potential function. This allowed him to construct a fourth order method. The potential function is replaced by a piecewise linear reference potential $\bar{V}(\delta) = F_0 + F_1\delta$. When we define $z(\delta) = F_1^{1/3}(\delta + F_0/F_1)$ and $z_0 = z(0)$, we have

$$u(\delta) \approx \bar{u}(\delta) = \pi\left[Bi'(z_0)Ai(z) - Ai'(z_0)Bi(z)\right] \tag{2.15}$$
$$u'(\delta) \approx \bar{u}'(\delta) = \pi F_1^{1/3}\left[Bi'(z_0)Ai'(z) - Ai'(z_0)Bi'(z)\right] \tag{2.16}$$
$$v(\delta) \approx \bar{v}(\delta) = \frac{\pi}{F_1^{1/3}}\left[-Bi(z_0)Ai(z) + Ai(z_0)Bi(z)\right] \tag{2.17}$$
$$v'(\delta) \approx \bar{v}'(\delta) = \pi\left[-Bi(z_0)Ai'(z) + Ai(z_0)Bi'(z)\right] \tag{2.18}$$

where Ai and Bi are the Airy functions. In the literature some improvements were described for the original method of Gordon mainly concerning the computation of the Airy functions which appear in the reference propagators (see e.g. [2, 27]). However, the intrinsic problem of linear coefficient approximation methods remained: they often suffer heavy accuracy losses due to the near-cancellation of similar terms. Instead of reducing to the constant approximation progagators, the linear approximation propagators in (2.15)-(2.18) blow up when $F_1 \to 0$, which causes severe near-cancellation effects. In [20], Ixaru suggested to use a perturbation procedure to rewrite the Airy propagators as combinations of η_{-1} and η_0 functions, eliminating all near-cancellation effects and avoiding the expensive and delicate evaluation of the Airy functions. Ixaru showed that if the reference potential is written as $V_0 + V_1 h P_1^*(\delta/h)$ where $P_1^*(\gamma) = -1 + 2\gamma$ is a shifted Legendre polynomial, then the following alternative formulae can be used for the Airy propagators in $\delta = h$ (only the values at $\delta = h$ are needed during propagation of the

solution):

$$\bar{u}(h) = \sum_{k=0}^{\infty} \frac{W^k}{k!} \left(\eta_{3k-1}(Z) - \frac{1}{2}\bar{V}_1 \eta_{3k+1}(Z) \right) \tag{2.19}$$

$$h\bar{u}'(h) = Z\eta_0(Z) + \sum_{k=1}^{\infty} \frac{W^k}{k!} \big(\eta_{3k-2}(Z) + (6k+1)\eta_{3k-1}(Z) \big) \tag{2.20}$$

$$\bar{v}(h) = h \sum_{k=0}^{\infty} \frac{W^k}{k!} \eta_{3k}(Z) \tag{2.21}$$

$$\bar{v}'(h) = \sum_{k=0}^{\infty} \frac{W^k}{k!} \left(\eta_{3k-1}(Z) + \frac{1}{2}\bar{V}_1 \eta_{3k+1}(Z) \right) \tag{2.22}$$

where $Z = (V_0 - E)h^2$, $\bar{V}_1 = V_1 h^3$, $W = -\bar{V}_1^2/24$ and the η functions as defined in the Appendix. When $V_1 \to 0$, the expressions in (2.19)-(2.22) tend to the constant approximation propagators in (2.11)-(2.14). This is not surprising, since equations (2.19)-(2.22) are obtained by solving the linear reference problem $y''(X+\delta) = [V_0 + V_1 h P_1^*(\delta/h) - E]y(X+\delta)$ in the so-called CP frame, that is with V_0 as the constant reference potential and $V_1 h P_1^*(\delta/h)$ as the perturbation from which correction terms are derived. This CP technique will be discussed in section 3. An infinite number of CP correction terms leads to the exact expressions for the linear approximation propagators (2.19)-(2.22). In practice, the infinite sums in (2.19)-(2.22) can be truncated at some suitable k-value determined by the order desired for the algorithm.

2.3. Coefficient approximation method based on higher degree polynomials

Due to the difficulties in obtaining the exact analytic expressions for their solutions, coefficient approximation methods based on piecewise parabolas or higher order polynomials, have not been considered in the literature. However, as suggested by Ixaru in [21], a perturbation approach can be used here to obtain the reference propagators in terms of the η functions, in a similar way as for the linear approximation method. This suggestion of Ixaru actually exactly corresponds to using piecewise perturbation to add correction terms to the constant (or linear) approximation method as is done in the so-called piecewise perturbation methods, which will be discussed next.

3. Piecewise perturbation methods

As for the methods described above, the original differential equation is replaced (piecewisely) by a reference equation which can be solved exactly. The idea underlying the Piecewise Perturbation Methods (PPM) is to use the perturbation theory to estimate the deviation between the solution of the reference equation and the solution of the original equation. Some perturbation corrections can then be added to the solution of the reference equation

to obtain a more accurate approximation to the solution of the original equation. The PPM are identified by the type of piecewise approximation used for the reference equation. If the coefficient $V(x)$ is approximated by piecewise constants the method is referred to as a CP method (or CPM) while if piecewise lines are used the method is called a LP method (or LPM).

3.1. The perturbation corrections

Our purpose is to construct the unknown propagators u and v of the original equation (2.3) in terms of the known reference propagators $\bar{u}$ and $\bar{v}$. Actually, the reference propagators form the "zeroth order" approximations of u and v and some perturbation corrections derived from the *perturbation*

$$\Delta_V(\delta) = V(X+\delta) - \bar{V}(X+\delta) \tag{3.1}$$

will successively improve this approximation. This perturbative procedure was discussed in [17]. The main result is given by the following theorem.

Theorem 3.1. *The solution of Eq.* (2.3) *with the initial conditions* $y(X) = \alpha$ *and* $y'(X) = \beta$ *can be written as Eq.* (2.8) *where the propagators* u *and* v *are written as perturbation series*

$$p(\delta) = p_0(\delta) + p_1(\delta) + p_2(\delta) + p_3(\delta) + \dots \tag{3.2}$$

where p *stands for* u *or* v*. The zeroth order propagator* $p_0(\delta)$ *is exactly the reference propagator* $\bar{p}(\delta)$ *and the* q*-th correction* $p_q(\delta)$, $q = 1, 2, 3, \dots$ *is the solution of the problem*

$$p_q'' = (\bar{V}(\delta) - E)p_q + \Delta_V(\delta)p_{q-1}, \quad p_q(0) = p_q'(0) = 0. \tag{3.3}$$

3.2. Computation of the perturbation corrections

One way to construct the perturbation corrections $p_q, q = 1, 2, \dots$ starts from the assumption that each p_q is a linear combination of the reference propagators and their first-order derivatives

$$p_q(\delta) = a_q\bar{u}(\delta) + b_q\bar{v}(\delta) + c_q\bar{u}'(\delta) + d_q\bar{v}'(\delta), \tag{3.4}$$

The functions a_q, b_q, c_q, d_q are determined by entering the expression (3.4) into (3.3), leading to the following system of differential equations:

$$\begin{aligned} a_q'' + 2c_q'(\bar{V} - E) + c_q\bar{V}' &= \Delta_V a_{q-1} \\ b_q'' + 2d_q'(\bar{V} - E) + d_q\bar{V}' &= \Delta_V b_{q-1} \\ c_q'' + 2a_q' &= \Delta_V c_{q-1} \\ d_q'' + 2b_q' &= \Delta_V d_{q-1} \end{aligned} \tag{3.5}$$

with initial conditions $a_q(0) + d_q(0) = 0$, $a_q'(0) + c_q(0)(\bar{V}(0) - E) + b_q(0) + d_q'(0) = 0$. When the potential $V(X+\delta)$ and the reference potential $\bar{V}(\delta)$ are polynomials in δ, the perturbation corrections can be evaluated analytically from (3.5). For $q = 1$, we have $a_0 = 1, b_0 = c_0 = d_0 = 0$ if $p = u$ and $b_0 = 1, a_0 = c_0 = d_0 = 0$ if $p = v$. This allows us to solve the system for a_1, b_1, c_1 and d_1; these are then introduced in the right hand sides of the system (3.5) for $q = 2$ and so on.

Equations (3.5) can be used to explicitly calculate the perturbation corrections, but for a constant reference function $\bar{V}$ the propagators and their derivative are connected via $\bar{u}' = (\bar{V} - E)\bar{v}$, $\bar{v}' = \bar{u}$ and the corrections can be searched for as a linear combination of the reference propagators alone. A slightly modified procedure is then usually prefered. The following theorem describes this procedure.

Theorem 3.2. *(Computation of the CPM perturbation corrections, from* [22]*). If the potential function $V(\delta)$ is a polynomial in δ, then the q-th correction p_q for the propagator $p = u, v$ is of the form*

$$p_q(\delta) = \sum_{m=0}^{\infty} C_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \tag{3.6}$$

$$p_q'(\delta) = C_0(\delta)\eta_{-1}(Z(\delta)) + \sum_{m=0}^{\infty} [C_m'(\delta) + \delta C_{m+1}(\delta)]\delta^{2m+1}\eta_m(Z(\delta)) \tag{3.7}$$

with a finite number of terms M, i.e. $C_m(\delta) = 0$ for $m > M$ and $Z(\delta) = (\bar{V} - E)\delta^2$. This means that the product $\Delta_V p_{q-1}$ is of the form

$$\Delta_V(\delta)p_{q-1}(\delta) = G(\delta)\eta_{-1}(Z(\delta)) + \sum_{m=0}^{\infty} S_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \tag{3.8}$$

and the coefficients $C_0(\delta), C_1(\delta), \ldots$ are then polynomials in δ which are given by quadrature

$$C_0(\delta) = \frac{1}{2}\int_0^{\delta} G(\delta_1)d\delta_1, \tag{3.9}$$

$$C_m(\delta) = \frac{1}{2}\delta^{-m}\int_0^{\delta} \delta_1^{m-1}[S_{m-1}(\delta_1) - C_{m-1}''(\delta_1)]d\delta_1, \quad m = 1, 2, \ldots \tag{3.10}$$

The starting functions in $\Delta_V u_0(\delta)$ are $G(\delta) = \Delta_V(\delta), S_0(\delta) = S_1(\delta) = \cdots = 0$, while for $\Delta_V v_0$ they are $G(\delta) = 0, S_0(\delta) = \Delta_V(\delta), S_1(\delta) = S_2(\delta) = \cdots = 0$.

Using this approach, a CPM perturbation correction is obtained in terms of the η functions (defined in the Appendix). Introducing these η functions gives us more transparent formulae for the correction terms which are more convenient for error control and step width adjustment. Unfortunaly, the procedure from theorem 3.2 cannot be extended to PPM with a non-constant $\bar{V}$, even not if the reference propagators are written in terms of the η functions, as for the linear reference propagators in (2.19)-(2.22). The reason is that $(\bar{V}(\delta) - E)\delta^2$ no longer equals the Z argument of the η-functions. In [27] and [21], the procedure (3.4)-(3.5) was followed to construct correction terms for the LPM.

3.3. A pilot reference equation

There is an intermediate stage in the procedure in which $V(X + \delta)$ is approximated by a polynomial in δ. This ensures that the system (3.3) has

an analytic solution. A good choice is to approximate the potential function $V(x)$ (piecewisely) by a series over shifted Legendre polynomials:

$$V(x_{i-1}+\delta) \approx \hat{V}(\delta) = \sum_{n=0}^{\nu-1} V_n h^n P_n^*(\delta/h), \quad \delta = x - x_{i-1}. \tag{3.11}$$

The function $\hat{V}$ is called the *pilot* reference function in [17]. The expressions of the first shifted Legendre polynomials $P_s^*(\gamma), \gamma \in [0,1]$ are as follows

$$P_0^*(\gamma) = 1, \;\; P_1^*(\gamma) = -1 + 2\gamma, \;\; P_2^*(\gamma) = 1 - 6\gamma + 6\gamma^2. \tag{3.12}$$

By the method of least squares the expressions for the coefficients V_n are obtained:

$$V_n = \frac{(2n+1)}{h^{n+1}} \int_0^h V(x_{i-1}+\delta) P_n^*(\delta/h) d\delta. \tag{3.13}$$

To compute the integrals (3.13), Gauss-Legendre quadrature of sufficient high order is used, i.e. to obtain an overall scheme of order 2ν, it is sufficient to take ν function evaluations of the potential function V. When the coefficients V_n are computed by such a ν-point Gauss-Legendre rule, the pilot reference potential (3.11) coincides with the Lagrange interpolation through the ν Legendre quadrature points. This can easily be verified for low values of ν.

3.4. Piecewise perturbation schemes

Depending on the number of correction terms included and the degree of the pilot reference polynomial $\hat{V}$, methods of different order can be constructed. In [17], fourth and sixth order CP schemes were introduced based on a second degree pilot reference function and one or two perturbation corrections. Higher order schemes (up to order sixteen) were presented in [22, 29] and implemented in the software packages SLCPM12 [23] and Matslise [30]. In [17, 21, 27] LP based schemes were constructed. It was noted in e.g. [21] that the LP algorithm presented "competes very well with a CP version of the same order" and that it has the advantage of "producing smaller errors when the potential function has a strong variation". In the next section, we will show, however, that the latter observation is not true since a CPM of a particular order is equivalent to a LPM of the same order leading to the same set of formulae when both are expressed in terms of η functions. Consequently, there is no advantage is using the one over the other. In fact, our main conlusion will be that there is no need to make a difference between (i) coefficient approximation methods without extra correction terms as we described them in section 2, (ii) CPM, (iii) LPM or (iv) methods based on higher degree reference potentials $\bar{V}$. When the reference propagators are expressed in terms of η functions to ensure their accurate and efficient computation, (i)-(iv) can be seen as just different approaches of obtaining the same numerical scheme.

4. Practical schemes

In this section, we will discuss the practical construction of some coefficient approximation schemes of different (even) order. Arbitrarely high order methods can be constructed. We first define the following parameters:

- $m = \nu - 1$: the degree of the piecewise polynomial approximations $\hat{V}$ in (3.11), sufficient to obtain a method of order $2m + 2$.
- K: the degree of the piecewise polynomial reference potential: $\bar{V}^{(K)}(\delta) = \sum_{n=0}^{K} V_n h^n P_n^*(\delta/h)$
- L: the number of different V_n in the perturbation $\Delta_V^{(K,m)}(\delta) = \hat{V}(\delta) - \bar{V}(\delta) = \sum_{n=K+1}^{m} V_n h^n P_n^*(\delta/h)$. These V_n-values will be brought into the numerical scheme through the correction terms. Note that $K + L = m$.

In theory, a method of order $2m + 2$ can be constructed in $m + 1$ ways, since $m + 1$ different values of K can be chosen: $K = 0, 1, \ldots, m$. As we will see, there is one prefered way, that is based on a constant reference potential ($K = 0$), leading to propagators expressed in terms of η functions.

4.1. Second order scheme

To obtain a second order method, it is sufficient to approximate the potential function by a piecewise constant approximation ($m = 0$). There is then only one option, namely $K = L = 0$. This means that the reference potential $\bar{V}$ equals $V_0 = \frac{1}{h}\int_0^h V(x_{i-1} + \delta)d\delta$ and no perturbation corrections need to be included. The one-node Gauss-Legendre quadrature rule suffices to compute the integral, giving us $\bar{V} = V(x_{i-1} + h/2)$. This corresponds to the constant approximation method from section 2.1.

4.2. Fourth order scheme

When the potential function $V(x_{i-1}+\delta)$ is approximated by a pilot reference potential of degree one, i.e. $\hat{V}(\delta) = V_0 + V_1 h P_1^*(\delta/h)$, a fourth order scheme can be obtained. In order to realize this fourth order scheme, we need to compute the expressions of the propagators $\hat{p} = \hat{u}, \hat{v}$ corresponding to the problem with the piecewise linear potential $\hat{V}$. This can be done in two ways, corresponding to the $K = 0, L = 1$ case and the $K = 1, L = 0$ case. The $K = 0$ option consists in using a piecewise constant reference potential $\bar{V}^{(0)} = V_0$ to construct the zeroth order propagators $p_0 = \bar{p}^{(0)}$ which then form a first approximation for the propagators $\hat{p}$:

$$\hat{p}(\delta) = p_0 + \sum_{k=1}^{\infty} p_k^{(0,1)}, \quad p = u, v. \tag{4.1}$$

Theorem 3.2 allows to compute the correction terms $\sum_{k=1}^{\infty} p_k^{(0,1)}$. Adding these correction terms ensures that the other part of the pilot reference potential, i.e. $\Delta_V^{(0,1)}(\delta) = V_1 h P_1^*(\delta/h)$ is also taken into account.

The $K = 1$ way of constructing $\hat{p}$ consists in taking a reference problem with a linear (reference) potential $\bar{V}^{(1)}(\delta) = \hat{V}(\delta)$ and using its exact solutions to form $\hat{p}$. This corresponds to Gordon's method. As mentioned in

section 2.2, the solutions of the reference problem with a piecewise linear potential can be expressed in terms of the Airy functions as in (2.15)-(2.18). Where the $K = 0$ (CPM) approach expresses $\hat{p}$ in (an infinite number of) η functions, the $K = 1$ (LPM) way leads thus to expressions of $\hat{p}$ in Airy functions. Assuming that an infinite number of correction terms can be taken in the $K = 0$ approach and that there are no computational problems in computing the Airy propagators in the $K = 1$ approach, both approaches return exact expressions for $\hat{p}$.

Of course, in practice, the series in (4.1) needs to be truncated. But this presents no problem since the infinite sum over perturbation contributions can be restricted to a relevant number of terms (determined by the order desired for the algorithm or the machine accuracy). In order to have a fourth order scheme, it is sufficient to retain only the terms proportional to $h^s, s \leq 4$. The notations $\bar{V}_n = V_n h^{n+2}, n = 1, 2, \ldots$ are used in PPM formulae expressed in terms of the η functions, since each V_n comes with a h^{n+2} factor, see e.g. [29]. Since $\bar{V}_1 \sim h^3$, only one perturbation correction term is needed to construct a fourth order scheme. A second correction term would lead to terms in $\bar{V}_1^2 \sim h^6$ and including them unaffects the order of the method (taking $m = 1$ limits the order to four), but can increase the accuracy of the method somewhat. The fourth order scheme with the minimal number of terms resulting when using the $K = 0$ approach is then (with $Z = Z(h) = (V_0 - E)h^2$):

$$u(h) \approx \eta_{-1}(Z) - \frac{\bar{V}_1}{2}\eta_1(Z) \tag{4.2}$$

$$v(h)/h \approx \eta_0(Z) \tag{4.3}$$

$$hu'(h) \approx Z\eta_0(Z) \tag{4.4}$$

$$v'(h) \approx \eta_{-1}(Z) + \frac{\bar{V}_1}{2}\eta_1(Z). \tag{4.5}$$

Let us again consider the $K = 1$ counterpart. The difficulties in practice with the propagators in terms of Airy functions are the near-cancellation effects and the efficient and accurate computation of the Airy functions themselves, which is time-consuming. As mentioned in section 2.2, this can be avoided by rewriting the Airy propagators in terms of the η functions. Ixaru obtained the alternative expressions (2.19)-(2.22) by applying a "constant perturbation" procedure with V_0 as constant reference potential and $V_1 h P_1^*(\delta/h)$ as the perturbation, which is actually the exact same thing as the $K = 0$ approach described above. Indeed, when one retains in (2.19)-(2.22) only the terms needed to construct a fourth order scheme, the same formulae as in (4.2)-(4.5) are obtained.

Figures 2 and 3 show some results obtained with different fourth order schemes based on a piecewise linear approximation of the potential for two typical test problems. The Mathieu problem is defined by

$$V(x) = 2\cos(2x), \quad y(0) = y(\pi) = 0, \tag{4.6}$$

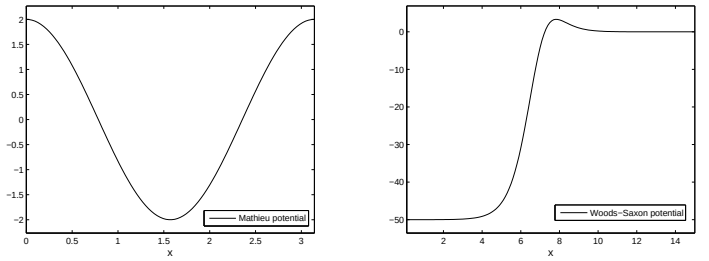

FIGURE 1. Potential functions $V(x)$ of the two test problems.

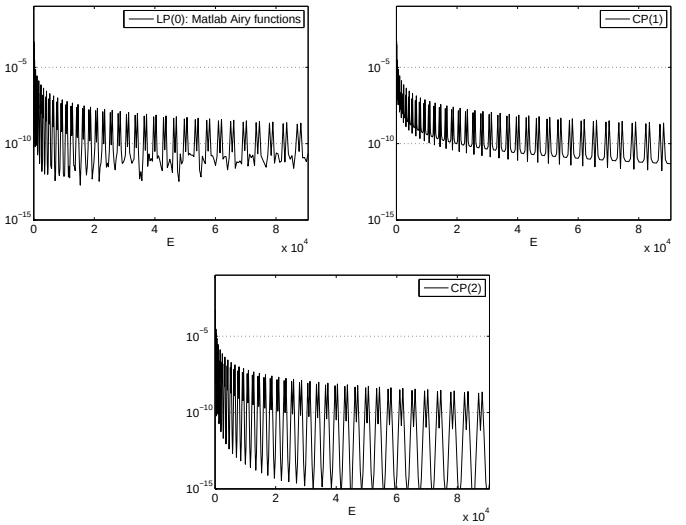

FIGURE 2. The Mathieu problem solved by different fourth order coefficient approximation schemes applied on an equidistant mesh with 8 steps. The plots show the error in $y(\pi)$ when the solution y is propagated from $x = 0$ to $x = \pi$ for the first 300 eigenvalues.

while the Woods-Saxon potential is

$$V(x) = v_0 w(x) \left(1 - \frac{1 - w(x)}{a_0}\right) \tag{4.7}$$

with $w(x) = (1+\exp((x-x_0)/a_0))^{-1}$, $v_0 = -50$, $x_0 = 7$, $a_0 = 0.6$ and defined on the truncated integration interval $x \in [0, 15]$. The potential functions of both problems are shown in Figure 1. Both problems have some variation in their potential.

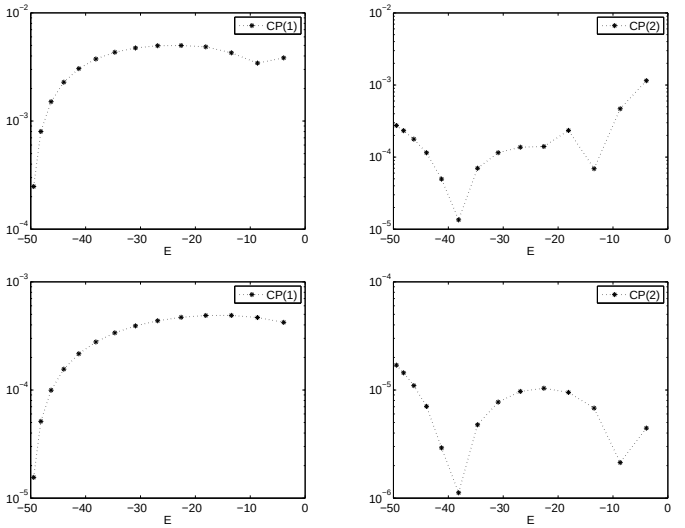

FIGURE 3. The Woods-Saxon problem solved by different fourth order coefficient approximation schemes. Equidistant meshes of 32 and 64 steps were used to construct the upper two, resp. lower two figures. The error in $y(0)$ is shown when the solution is propagated from $x = 15$ to $x = 0$ with initial conditions $y(15) = 0, y'(15) = 1$ for the 14 eigenvalues.

Different fourth order schemes were applied to construct the figures 2 and 3. A first method, denoted by LP(0), consists in the use of reference propagators expressed in terms of the Airy functions as in the formulae (2.15)-(2.18), no correction terms are added. This method suffers from accuracy losses, as seen on the first plot for the Mathieu problem and even fails completely for the Woods-Saxon problem due to heavy near-cancellation effects and blow-up problems, which is why no plot is included for this problem.

The CP(1) method in the figures 2 and 3 consists in the application of a CP approach with one correction term, i.e. the method listed in (4.2)-(4.5). As mentioned, the accuracy of this method can be increased by adding more correction terms. The CP(2) method is the scheme where a second correction term is added to the CP scheme, or equivalently the scheme where also $\bar{V}_1^2$

terms are retained from (2.19)-(2.22):

$$u(h) \approx \eta_{-1}(Z) - \frac{\bar{V}_1}{2}\eta_1(Z) - \frac{\bar{V}_1^2}{24}\eta_2(Z) \tag{4.8}$$

$$v(h)/h \approx \eta_0(Z) - \frac{\bar{V}_1^2}{24}\eta_3(Z) \tag{4.9}$$

$$hu'(h) \approx Z\eta_0(Z) - \frac{\bar{V}_1^2}{24}\eta_1(Z) + 7\frac{\bar{V}_1^2}{24}\eta_2(Z) \tag{4.10}$$

$$v'(h) \approx \eta_{-1}(Z) + \frac{\bar{V}_1}{2}\eta_1(Z) - \frac{\bar{V}_1^2}{24}\eta_2(Z). \tag{4.11}$$

Adding the $\bar{V}_1^2$ to the algorithm does not change the order of the method but indeed increases the accuracy for our test problems (and this without computing more function evaluations of the potential). Adding more correction terms, e.g. the terms in $\bar{V}_1^3$ and $\bar{V}_1^4$ have only minor influence on the accuracy of the method for these testproblems.

It is clear that the CP-based methods should be prefered to be applied in practice. As seen for the two test problems here, the number of correction terms which lead to an increase in accuracy is limited. The contribution of a correction term is decreasing with its order and a substantial small number of terms is usually sufficient to reach machine accuracy in approximating $\hat{p}$. Moreover, next to the error caused by truncating the infinite number of correction terms, there is also the error caused by approximating the potential by the linear potential $\hat{V}$. At some point the latter error will be larger than the error induced by not taking into account more correction terms.

4.3. Sixth order scheme

In order to obtain a sixth order method, the potential needs to be approximated by a piecewise polynomial of degree (at least) two: $V(x_{i-1}\delta) \approx \hat{V}(\delta) = V_0 + \sum_{l=1}^{2} V_l h P_l^*(\delta/h)$. The following options exist to compute the propagators $\hat{p}$ corresponding to this approximating potential: (i) $K = 0, L = 2$, (ii) $K = 1, L = 1$ or (iii) $K = 2, L = 0$.

The CPM approach (i.e. $K = 0$) takes a piecewise constant reference potential $\bar{V}^{(0)} = V_0$ and computes extra correction terms to add to the known solution of the reference problem. The quantities $\bar{V}_l h^{l+2}, l = 1, 2 = L$ appear in the correction terms. Since only the terms in $O(h^s), s \leq 6$ need to be retained, only two corrections need to be taken. The following sixth order

scheme results

$$u(h) \approx \eta_{-1}(Z) - \frac{\bar{V}_1}{2}\eta_1(Z) - \frac{\bar{V}_1^2}{24}\eta_2(Z) + \left\{ \frac{\bar{V}_1\bar{V}_2}{2}\eta_3(Z) - \frac{\eta_2(Z)+3\eta_3(Z)}{40}\bar{V}_2^2 \right\} \tag{4.12}$$

$$v(h)/h \approx \eta_0(Z) - \frac{\bar{V}_2}{2}\eta_0(Z) - \frac{\bar{V}_1^2}{24}\eta_3(Z) - \left\{ \frac{\eta_3(Z)-9\eta_4(Z)}{40}\bar{V}_2^2 \right\} \tag{4.13}$$

$$hu'(h) \approx Z\eta_0(Z) + \frac{\bar{V}_2}{2}\eta_0(Z) - \left[\frac{3}{2}\bar{V}_2 + \frac{\bar{V}_1^2}{24}\right]\eta_1(Z) - \frac{7}{24}\bar{V}_1^2\eta_2(Z) - \left\{ \frac{\eta_1(Z)+6\eta_2(Z)-57\eta_3(Z)}{40}\bar{V}_2^2 \right\} \tag{4.14}$$

$$v'(h) \approx \eta_{-1}(Z) + \frac{\bar{V}_1}{2}\eta_1(Z) - \frac{\bar{V}_1^2}{24}\eta_2(Z) - \left\{ \frac{\bar{V}_1\bar{V}_2}{2}\eta_3(Z) - \frac{\eta_2(Z)+3\eta_3(Z)}{40}\bar{V}_2^2 \right\} \tag{4.15}$$

The terms between curly brackets can be included to obtain a better accuracy, but are not needed to attain a sixth order scheme.

The formulae (4.12)-(4.15) are also obtained for $K = 1$ when one truncates the expressions (2.19)-(2.22) for the reference propagators $\bar{p}^{(1)}$ and one uses the perturbation technique (3.4)-(3.5) with $\bar{V}^{(1)} = V_0 + V_1 h P_1^*(\delta/h)$ and $\Delta_V^{(1,2)}(\delta) = V_2 h^2 P_2^*(\delta/h)$ to construct correction terms $p_q^{(1,2)}$. Equations (3.4)-(3.5) give us, for example, the following expression for the first correction in $u(h)$ (see [21])

$$u_1^{(1,2)}(h) = \frac{3\bar{V}_2}{\bar{V}_1}\Big[-\frac{\bar{u}^{(1)}(h)}{5} + \left(\frac{1}{5} - 2\bar{V}_1 QS\right)\frac{\bar{v}^{(1)}(h)}{h} + \left(S - \frac{2}{15}(1+2Q)\right)h\bar{u}^{(1)'}(h)\Big] \tag{4.16}$$

with

$$Q = \frac{Z}{2\bar{V}_1} - \frac{1}{2}, \quad S = \frac{1}{6} + \frac{2Q}{3}\left(1 + \frac{4}{5}Q\right), \quad Z = (V_0 - E)h^2.$$

Introducing the expressions (2.19)-(2.22) gives

$$u_1^{(1,2)}(h) = \frac{\bar{V}_2}{\bar{V}_1}\Big[-\frac{3}{5}\eta_{-1}(Z) + \frac{1}{5}\left(Z - \frac{\bar{V}_1}{2} + 3\right)\eta_0(Z) + \frac{1}{10}\left(3\bar{V}_1 + \frac{\bar{V}_1^2}{24} + \frac{Z\bar{V}_1}{12} - \frac{Z^2}{6}\right)\eta_1(Z) - \frac{7}{60}\left(Z^2 - \frac{13\bar{V}_1^2}{28} - \frac{Z\bar{V}_1}{2}\right)\eta_2(Z) + \frac{1}{20}\left(\frac{\bar{V}_1^3}{12} - \frac{Z\bar{V}_1^2}{4} + \frac{Z^3}{3} - \frac{Z^2\bar{V}_1}{6} - \frac{\bar{V}_1^2}{2}\right)\eta_3(Z) + \dots\Big] \tag{4.17}$$

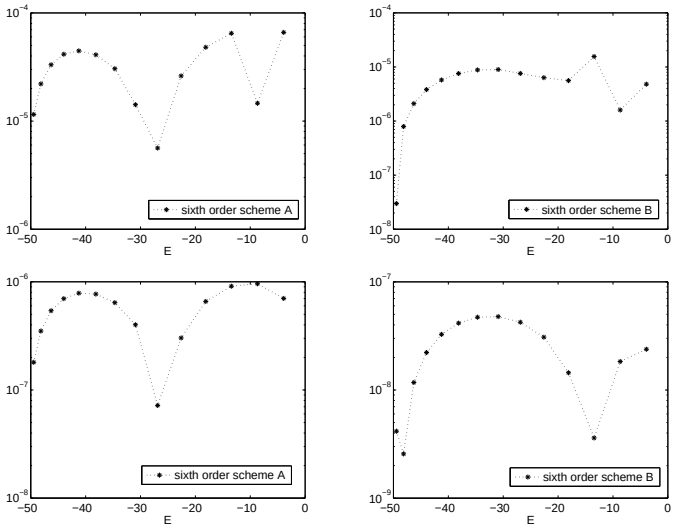

FIGURE 4. The Woods-Saxon problem solved by the sixth order scheme (4.12)-(4.15), (A) without and (B) with the terms between curly braces. Equidistant meshes of 32 and 64 steps were used for the upper, resp. lower figures. The error in $y(0)$ is shown when the solution is propagated from $x = 15$ to $x = 0$ for the 14 eigenvalues.

To remove all difficulties when $\bar{V}_1 \to 0$, we have to use the identities (A.3) at the appropriate places in (4.17) to obtain

$$u_1^{(1,2)}(h) = \frac{\bar{V}_1 \bar{V}_2}{2} \eta_3(Z) + (\dots)\eta_4(Z) + \dots$$

It is clear that the direct CP approach ($K = 0$), where correction terms are computed via (3.6)-(3.10), immediately results in the most appropriate form, whereas for $K = 1$ this is not true. For $K > 0$ values the obtained expressions for the correction terms can be reduced to a similar CP form but this process can be far from trivial. Also for option (iii) ($K = 2$) computing the solutions of a Schrödinger problem with a piecewise second degree polynomial potential is not trivial and a perturbation procedure should be used to compute expressions for these solutions, where V_0 is taken as constant reference function to form first approximations and correction terms are computed from the perturbation $\sum_{l=1}^{2} V_l h P_l^*(\delta/h)$. This approach corresponds, in fact, to option (i) and again formulae (4.12)-(4.15) can be derived.

Figure 4 shows some results for the Woods-Saxon problem.

4.4. Higher order methods

Methods of higher order can be developed using a similar approach as described above for the fourth and sixth order algorithm. Approximating the

potential piecewisely by a pilot reference polynomial $\hat{V}$ of degree three, leads to a method of order eight when one takes a sufficient number of correction terms. Order ten is reached for a pilot potential of degree four, order twelve for a pilot potential of degree five and so on.

In general, the potential is approximated over the current mesh interval by $\hat{V}(\delta) = \sum_{n=0}^{m} V_n h^n P_n^*(\delta/h)$ and a reference potential of degree $K, 0 \leq K \leq m$ is taken: $\bar{V}^{(K)}(\delta) = \sum_{n=0}^{K} V_n h^n P_n^*(\delta/h)$. The propagator, denoted here as $\hat{p} = \hat{u}, \hat{v}$, is constructed as the sum of the reference propagator $\bar{p}^{(K)}$ and some correction terms $p_q^{(K,m)}$:

$$\hat{p} = \bar{p}^{(K)} + \sum_{q=1}^{\infty} p_q^{(K,m)}.$$

The notation $p_q^{(K,m)}$ is used to denote the qth correction term derived from the perturbation $\Delta_V^{(K,m)}(\delta) = \sum_{n=K+1}^{m} V_n h^n P_n^*(\delta/h)$.

The choice $K = 0$ corresponds to the CP approach. This means that the reference propagator is given here by $\bar{p}^{(0)} = \eta_{-1}(Z(\delta))$ for $p = u$ and $\bar{p}^{(0)} = \delta\eta_0(Z(\delta))$ for $p = v$ and the propagator $\hat{p}$ is computed as

$$\hat{p} = \bar{p}^{(0)} + \sum_{q=1}^{\infty} p_q^{(0,m)}. \tag{4.18}$$

The correction terms $p_q^{(0,m)}$ are explicitly evaluated in terms of the η functions using the procedure described in theorem 3.2.

When K is larger than zero, the only practical way to compute the reference propagator $\bar{p}^{(K)}$ is by using a (constant) perturbation procedure. This extra perturbation procedure avoids the numerical difficulties/instabilities in the computation of the (Airy) reference propagator for $K = 1$ and resolves the issue that the analytic expressions for the $K > 1$ reference propagators are difficult to obtain. $\bar{p}^{(K)}$ is then constructed as

$$\bar{p}^{(K)} = \bar{p}^{(0)} + \sum_{q=1}^{\infty} p_q^{(0,K)}$$

Adding the correction terms, gives us the following formula for the propagators of the $K > 0$ scheme:

$$\hat{p} = \bar{p}^{(0)} + \sum_{q=1}^{\infty} p_q^{(0,K)} + \sum_{q=1}^{\infty} p_q^{(K,m)}. \tag{4.19}$$

Theorem 4.1. *When the propagator $\hat{p}$ corresponding to the polynomial potential $\hat{V}$ is constructed as the sum of the reference propagator $\bar{p}^{(K)}$ and some correction terms $p_q^{(K,m)}$:*

$$\hat{p} = \bar{p}^{(K)} + \sum_{q=1}^{\infty} p_q^{(K,m)},$$

equivalent formulae are obtained for all possible choices of K.

Proof. Since infinite numbers of corrections terms are taken, approach (4.18) and approach (4.19) give us exact expressions for $\hat{p}$, or equivalently $\sum_{q=1}^{\infty} p_q^{(0,m)} = \sum_{q=1}^{\infty} p_q^{(0,K)} + \sum_{q=1}^{\infty} p_q^{(K,m)}$. In practice, terms of degree in h larger than a certain value P are ignored and consequently a small number of correction terms is usually sufficient. For instance, $\sum_{q=1}^{\infty} p_q^{(0,m)}$ and $\sum_{q=1}^{\infty} p_q^{(0,K)}$ for $p = u$ can be truncated at $q = \lfloor P/3 \rfloor$, while going upto $q = \lfloor P/(K+1+2) \rfloor$ is sufficient for $\sum_{q=1}^{\infty} p_q^{(K,m)}$. When in the exact expressions for both approaches the same powers of h are ignored, the resulting formulae are of course still equivalent. Consequently, when the relations (A.3) are used to reduce the resulting formulae for both approaches to a form $A(Z)\eta_{-1}(Z) + B(Z)\eta_0(Z)$, $Z = (V_0 - E)\delta^2$, exactly the same A and B will be obtained for both approaches. □

For practical purposes, it is preferable to have the formulae for $\hat{p}$ in the specific form

$$\hat{p} = \sum_{s=-1}^{S} C_s \eta_s(Z) \tag{4.20}$$

where the C coefficients depend only on $\bar{V}_1, \bar{V}_2, \ldots \bar{V}_m$ while the energy dependent Z appears only as argument of the η functions. In this way, numerical difficulties such as near-cancellation effects are avoided and a fast evaluation of $\hat{p}$ is made possible: the C_s coefficients can be computed once and stored for repeated re-use during a shooting process, only the values of $\eta_s(Z)$ need to be updated at each new E value but their computation is fast. In this respect, approach (4.18) is the most suitable way to construct a PPM scheme since the correction terms are brought in the desired form (4.20) already through the procedure described in theorem 3.2. Approach (4.19) on the other hand, needs two different techniques to construct expressions for the correction terms $p_q^{(0,K)}$ and $p_q^{(K,m)}$. The process of solving the set of differential equations to obtain $p_q^{(K,m)}$ is not obvious, especially for larger K and q values and extra effort is needed to write each $p_q^{(K,m)}$ into the form (4.20). Moreover the technique of constructing correction terms $p_q^{(K,m)}$ via (3.4)-(3.5) is difficult to automatize in a symbolic software code which can be used for different K or m values, whereas a Maple-code exists which can generate formulae for the CP corrections $p_q^{(0,m)}$ for any m (see [29]).

4.5. Note on $\{P,P_{as}\}$ schemes

As mentioned above, methods of arbitrarely high order can be developed. With the term "order" we mean the order of the method as it has its counterpart when dealing with the classical numerical methods (multistep, Runge-Kutta). That is, when the order of the method is P, the one-step error behaves as h^{P+1} when $|Z|$ is small. To coefficient approximation methods one can, however, associate also an asymptotic order P_{as}. The error for these methods decreases as E is increased and the one-step error behaves as $h^{P_{as}+1}/\sqrt{E}$ when $-Z \to \infty$, i.e. at high (asymptotic) energies E (see [22]). The notation

CPM{P,P_{as}} was introduced to denote a CPM scheme with order P and asymptotic order P_{as}. In [22] a CPM{12,10} method was described and in [21] a LPM counterpart has been presented. The formulae of the LPM{12,10} scheme from [21] equal the CPM{12,10} ones apart from some small modifications: (i) some terms in h^{13} and h^{14} are also retained and (ii) the expressions $(\bar{V}_1 + \bar{V}_3 + \bar{V}_5 + \bar{V}_7 + \bar{V}_9)/2$ and $(\bar{V}_2 + \bar{V}_4 + \bar{V}_6 + \bar{V}_8 + \bar{V}_{10})/2$ which appear in the CPM formulae and in fact equal $h^2[\hat{V}(X) - \hat{V}(X+h)]/4$ and $h^2[\hat{V}(X) + \hat{V}(X+h) - 2V_0]/4$ resp., are replaced by the "exact" expressions $h^2[V(X) - V(X+h)]/4$ and $h^2[V(X) + V(X+h) - 2V_0]/4$, requiring an extra function evaluation for each mesh interval. These modifications do not change the order of the method but make the method a bit more accurate (but also a bit more expensive), just as the scheme (4.8)-(4.11) is more accurate than the other fourth order scheme (4.2)-(4.5). The modifications are not intrinsic to the LP method, and could equally well be added to the CPM{12,10} scheme. The slightly better performance of the LPM{12,10} algorithm from [21] should thus not be attributed to the fact that linear ($K = 1$) reference potentials $\bar{V}$ are used instead of constant ($K = 0$) reference potentials $\bar{V}$ and that these present a better approximation of the potential V. If the same pilot reference potential $\hat{V}$ is used and terms are retained upto the same power in h, both LP and CP approach will lead to the same scheme. Also piecewise perturbation methods of order {12,10} based on piecewise parabolas or higher order piecewise reference polynomials $\bar{V}$ would be equivalent to the CPM{12,10} scheme. In the conclusion of [21], it was written that "the treatment in this way of a method based on piecewise parabolas may be of acute importance". With "in this way", Ixaru meant to construct expressions for the reference propagators $\bar{p}$ using a CP approach, i.e. with V_0 and $\bar{V} - V_0$ as the reference potential and the perturbation resp., and to use these expressions to start computing correction terms from. However, this will lead us again to the same CPM{12,10} formulae.

5. Conclusion

If in the construction of a piecewise perturbation method (PPM), the potential V is approximated by a (pilot reference) polynomial of degree m of the form $V \approx \hat{V} = \sum_{s=0}^{m} V_s h^s P_s^*(\delta/h)$, it doesn't matter which K value one takes to form the reference potential $\bar{V} = \sum_{s=0}^{K} V_s h^s P_s^*(\delta/h)$ as long as the remaining part of $\hat{V}$, i.e. the perturbation $\Delta_V(\delta) = \sum_{s=K+1}^{m} V_s h^s P_s^*(\delta/h)$, is taken into account in the form of correction terms. When an infinite number of correction terms are taken, all approaches corresponding to different choices of K give exact expressions for the propagators $\hat{p}, (p = u, v)$ corresponding to the pilot reference problem. In practice, only a limited number of perturbation corrections can be taken into account for all different PPM versions ($K = 0, 1, \dots$) and the number of terms is determined by the order of the algorithm one is constructing. Since for $K > 0$, one experiences difficulties in the computation of the reference propagators $\bar{p}$, one is forced

to use specialized techniques. One way is to reexpress the reference propagators in terms of η functions, and in that case one eventually obtains exactly the same formulae for $\hat{p}$ as when one constructs a CPM ($K = 0$), but less directly. There is consequently no reason to distinguish different classes of piecewise perturbation methods or to prefer $K > 0$ schemes over CP methods for some types of potentials. We can conclude that PPM=CPM=LPM, when we consider them in a form which is the most convenient in practice. When it comes to the construction of practical schemes, the way to construct a coefficient approximation method of a particular order is by using a constant reference potential $\bar{V} = V_0$ and computing correction terms from the perturbation $\Delta_V = \hat{V} - V_0$ by the procedure described in Theorem 3.2.

Appendix A

The functions $\eta_{-1}(Z), \eta_0(Z), \eta_1(Z), \ldots$, originally introduced in [17] (they are denoted there as $\bar{\xi}(Z), \bar{\eta}_0(Z), \bar{\eta}_1(Z), \ldots$), are defined as follows :

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0\,, \\ \cosh(Z^{1/2}) & \text{if } Z > 0\,, \end{cases} \tag{A.1}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0\,, \\ 1 & \text{if } Z = 0\,, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0\,, \end{cases} \tag{A.2}$$

and

$$\begin{aligned} \eta_1(Z) &= [\eta_{-1}(Z) - \eta_0(Z)]/Z \\ \eta_m &= [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z\,, \quad m = 2, 3, \ldots \end{aligned} \tag{A.3}$$

The functions obey the following differentiation properties :

$$\eta'_{-1}(Z) = \frac{1}{2}\eta_0(Z)\,, \quad \eta'_m(Z) = \frac{1}{2}\eta_{m+1}(Z)\,,\ m = 0, 1, 2, \ldots \tag{A.4}$$

References

[1] M. Abramowitz and I. A. Segun. *Handbook of Mathematical Functions*. Dover, 1965.

[2] M. H. Alexander and D. E. Manolopoulos. A stable linear reference potential algorithm for solution of the quantum close-coupled equations in molecular scattering theory. *J. Chem. Phys.*, **86** (1987), 2044–2050.

[3] A. L. Andrew. Twenty years of asymptotic correction for eigenvalue computation. *ANZIAM J.*, **42** (2000), C96-C116.

[4] A. Arnold, N. Ben Abdallah and C. Negulescu. WKB-based schemes for the Schrödinger equation in the semi-classical limit. preprint (2010).

[5] N. Ben Abdallah, C. Negulescu and M. Mouis. An accelerated algorithm for 2D simulations of the quantum ballistic transport in nanoscale MOSFETs. *J. Comput. Phys.*, **225** (2007), 74–99.

[6] N. Ben Abdallah, and O. Pinaud. Multiscale simulation of transport in an open quantum system: Resonances and WKB interpolation. *J. Comput. Phys.*, **213** (2006), 288–310.

[7] J. Canosa and R. G. De Oliveira. A new method for the solution of the Schrödinger equation. *J. Comput. Phys.*, **5** (1970), 188–207.

[8] I. Degani and J. Schiff. RCMS: Right Correction Magnus Series approach for oscillatory ODEs. *J. Comput. Appl. Math*, **193** (2006), 413–436.

[9] R. G. Gordon. New method for construcing wavefunctions for bound states and scattering. *J. Chem. Phys.*, **51** (1969), 14–25.

[10] L. Greenberg and M. Marletta. Oscillation theory and numerical solution of 4th-order Sturm-Liouville problems *IMA J. Numer. Anal.*, **15** (1995), 319–356.

[11] L. Greenberg and M. Marletta. Algorithm 775: The code SLEUTH for solving fourth-order Sturm-Liouville problems *ACM. Trans. Math. Software*, **23** (1997), 453–493.

[12] L. Greenberg and M. Marletta. Oscillation theory and numerical solution of sixth order Sturm-Liouville problems *SIAM J. Numer. Anal.*, **35** (1998), 2070–2098.

[13] A. Iserles. Think globally, act locally: solving highly-oscillatory ordinary differential equations *BIT*, **43** (2004), 145–160.

[14] A. Iserles. On the method of Neumann series for highly oscillatory equations. *BIT*, **44** (2004), 473–488.

[15] A. Iserles. On the numerical quadrature of highly-oscillating integrals I: Fourier transforms. *IMA J. Num. Anal.*, **24** (2004), 365–391.

[16] L. Gr. Ixaru. The error analysis of the algebraic method for solving the Schrödinger equation. *J. Comput. Phys.*, **9** (1972), 159–163.

[17] L. Gr. Ixaru. *Numerical Methods for Differential Equations and Applications.* Reidel, 1984.

[18] L. Gr. Ixaru. CP methods for the Schrödinger equation. *J. Comput. Appl. Math.*, **125** (2000), 347–357.

[19] L. Gr. Ixaru. LILIX - A package for the solution of the coupled channel Schrödinger equation. *Comput. Phys. Commun.*, **147** (2002), 834–852.

[20] L. Gr Ixaru. Efficient computation of the Airy propagators. *Comput. Phys. Commun.*, **176** (2007), 637–641.

[21] L. Gr Ixaru. Fast LP method for the Schrödinger equation. *Comput. Phys. Commun.*, **177** (2007), 897–907.

[22] L. Gr. Ixaru, H. De Meyer, and G. Vanden Berghe. CP methods for the Schrödinger equation, revisited. *J. Comput. Appl. Math.*, **88** (1997), 289–314.

[23] L. Gr. Ixaru, H. De Meyer, and G. Vanden Berghe. SLCPM12 - a program for solving regular Sturm-Liouville problems. *Comput. Phys. Commun.*, **118** (1999), 259–277.

[24] L. Gr. Ixaru. New numerical method for the eigenvalue problem of the 2D Schrödinger equation. *Comput. Phys. Commun.*, **181** (2010), 1738–1742.

[25] T. Jahnke and C. Lubich. Numerical integrators for quantum dynamics close to the adiabatic limit. *Numer. Math.*, **94** (2003), 289–314.

[26] T. Jahnke. Long time step integrators for almost adiabatic quantum dynamics. *SIAM J. Sci. Comput.*, **25** (2004), 2145–2164.

[27] V. Ledoux, M. Rizea, L. Gr Ixaru, G. Vanden Berghe, and M. Van Daele. Solution of the Schrödinger equation by a high order perturbation method based on a linear reference potential. *Comput. Phys. Commun.*, **175** (2006), 424–439.

[28] V. Ledoux, M. Rizea, L. Gr Ixaru, M. Van Daele, G. Vanden Berghe and I. Silisteanu. Eigenvalue problem for a coupled channel Schrödinger equation with application to the description of deformed nuclear systems. *J. Comput. Appl. Math.*, **228** (2009), 197–211.

[29] V. Ledoux, M. Van Daele, and G. Vanden Berghe. CP methods of higher order for Sturm-Liouville and Schrödinger equations. *Comput. Phys. Commun.*, **162** (2004), 151–165.

[30] V. Ledoux, M. Van Daele, and G. Vanden Berghe. Matslise: A matlab package for the numerical solution of Sturm-Liouville and Schrödinger equations. *ACM Trans. Math. Software*, **31** (2005), 532–554.

[31] V. Ledoux, M. Van Daele, and G. Vanden Berghe. CPM{P,N} methods extended for the solution of coupled channel Schrödinger equations. *Comp. Phys. Commun.*, **174** (2006), 357–370.

[32] V. Ledoux, M. Van Daele, and G. Vanden Berghe. Efficient numerical solution of the 1D Schrödinger eigenvalue problem using Magnus integrators. *IMA J. Num. Anal.*, **30** (2010), 751–776.

[33] V. Ledoux, M. Van Daele. Solving Sturm-Liouville problems by piecewise perturbation methods, revisited. *Comp. Phys. Commun.*, **181** (2010), 1335–1345.

[34] M. Marletta and J. D. Pryce. Automatic solution of Sturm-Liouville problems using the Pruess method. *J. Comput. Appl. Math.*, **39** (1992), 57–78.

[35] L. F. Shampine and G. Kraut. Uniformly Accurate Sturm-Liouville Eigenvalues. *Computing*, **47** (1992), 379–385.

[36] J. W. Paine and F. R. de Hoog. Uniform estimation of the eigenvalues of Sturm-Liouville problems. *J. Austral. Math. Soc. Ser. B*, **21** (1980), 365–383.

[37] S. Pruess. Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equation. *SIAM J. Numer. Anal.*, **10** (1973) 55–68.

[38] S. Pruess. High-order approximations to Sturm-Liouville eigenvalues. *Numer. Math.*, **24** (1975), 241–247.

[39] S. Pruess and C. T. Fulton. Mathematical software for Sturm-Liouville problems. *ACM Trans. Math. Software*, **19** (1993), 360–376.

[40] J. D. Pryce. *Numerical Solution of Sturm-Liouville Problems*. Oxford University Press, 1993.

[41] J. D. Pryce and M. Marletta. A new multipurpose software package for Schrödinger and Sturm-Liouville computations. *Comp. Phys. Commun.*, **62** (1991), 42–52.

[42] M. D. Smooke. Piecewise analytical perturbation series solutions of the radial Schrödinger equation: one-dimensional case. *SIAM J. Sci. Stat. Comput.*, **3** (1982), 195–222.

[43] G. Vanden Berghe and H. De Meyer. Accurate computation of higher Sturm-Liouville eigenvalues. *Numer. Math.* , **59** (1991), 243–254.

Veerle Ledoux
Vakgroep Toegepaste Wiskunde en Informatica
Ghent University
Krijgslaan 281-S9
B-9000 Gent
Belgium
e-mail: Veerle.Ledoux@UGent.be

Marnix Van Daele
Vakgroep Toegepaste Wiskunde en Informatica
Ghent University
Krijgslaan 281-S9
B-9000 Gent
Belgium
e-mail: Marnix.VanDaele@UGent.be